

# Implications of Modeling for Gas-Phase Transport at the LLNL Vadose Zone Observatory

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Transport by the gas phase represents a potential mode by which contaminants can spread throughout the vadose zone and ultimately reach the underlying water table. In addition to spreading contamination, movement of the gas phase can also influence estimates of contaminant inventories that are based upon gas sampling at different levels in a monitoring well. Using the NUFT multiphase flow-and-transport code, we have carried out calculations that include the effect of barometric pumping upon gas-phase transport in a variety of subsurface soil distributions with and without fractures. In particular, we have attempted to model a soil regime similar to that characterizing the LLNL Vadose Zone Observatory (VZO). Most previous work examining barometric pumping has used models that address only vertical contaminant transport. The present calculations model both vertical and horizontal transport by pumping. A degree of irreversibility in the subsurface pumping process can enhance the spread of contamination. Potential mechanisms for introducing irreversibility over many cycles include mechanical dispersion, chemical diffusion, or chemical reaction. Although we find marginal enhancements (< 10 percent) of transport from barometric pumping compared with gas-phase diffusion alone, to date our models of unfractured soils do not show that barometric pumping is a particularly effective mass transport mechanism in the vadose zone. Indeed, gas-tracer experiments carried out at the VZO appear to be consistent with a heterogeneous, silt-and-sand soil distribution that is nearly diffusion dominated. Our models do suggest that barometric pressure fluctuations can strongly influence estimates of the subsurface contaminant inventory that are based on gas sampling. This work was performed under the auspices of the U.S. Department of Energy by the Lawrence Livermore National Laboratory under contract number W-7405-ENG-48.

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